

The Kirchhoff Rod as a XY Spin Chain Model

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Abstract. A XY Heisenberg spin chain model with two perpendicular spins per site is mapped onto a Kirchhoff thin elastic rod. It is shown that in the case of constant curvature the Euler–Lagrange equation leads to the static sine-Gordon equation. The kink-antikink type and periodical static solutions for these models are derived.

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1. Introduction

The study of an elastic rods [1] is a subject to increased interest [2, 3, 4, 5, 6, 7, 8] especially in connection with the biomathematical models of proteins and of DNA [9, 10]. The main feature of a thin rod is a space curve (rod's axis) and the corresponding orthonormal frame with a tangent vector \mathbf{t} to the axial curve. The static energy of the elastic rod is related to the bending and twisting energies. It is tempting to map the elastic rod problem to a classical spin chain [11] (in the continuum limit, where the normalized spin \mathbf{S} is mapped onto the tangent vector \mathbf{t}). We will show however that the full mapping of the elastic rod onto a spin-chain model requires a system of two orthogonal spins.

The spin Hamiltonian for a Heisenberg spin chain is given by the following expression:

$$H = J_0 \sum_i \mathbf{S}_i(s) \cdot \mathbf{S}_{i+1}(s), \quad \mathbf{S}_i^2 = \mathbf{S}_{i+1}^2 = 1. \quad (1)$$

In the continuum limit this Hamiltonian goes over to

$$H = J_0 \int_{-\infty}^{+\infty} \left(\frac{d\mathbf{S}(x)}{dx} \right)^2 dx. \quad (2)$$

In the case of XY spin chain the spin is given by the rotation angle $\theta(x)$: $\mathbf{S}(s) = (\cos \theta(x), \sin \theta(x))$. The Hamiltonian now reads $H = J_0 \int_{-\infty}^{+\infty} \left(\frac{d\theta}{dx} \right)^2 dx$.

This letter is organized as follows: In section 2 are discussed the static properties of the Kirchhoff equations for a thin elastic rod. It is shown that if a curvature is present the twist angle satisfies the static sine-Gordon equation. The mapping of the Kirchhoff model onto a XY spin chain is done in Section 3. In Section 4 the soliton-like solutions for the static sine-Gordon equations are briefly discussed.

2. Kirchhoff Model for Elastic Rods

The model introduced by Kirchhoff (1859) describes the shape and the dynamics of a thin elastic rod in equilibrium and is based on the analogy with the dynamics of a heavy spinning top (the Lagrange case). The shape is described by the *static Kirchhoff model* while the time evolution – by the *dynamical Kirchhoff model*. Here we will concentrate on the statics of thin elastic rods (here and below we shall call them Kirchhoff rods).

We consider a static space curve $\mathbf{R}(s) : \mathbb{R} \rightarrow \mathbb{R}^3$ as a smooth function mapping the arc-length interval $I \subset \mathbb{R}$ into the physical space \mathbb{R}^3 . For every s we define the Frenet basis $(\mathbf{t}(s), \mathbf{n}(s), \mathbf{b}(s))$ to be the normal, binormal and the tangent vectors to the curve(s). The tangent vector is a unit vector given by $\mathbf{t} = (\frac{d\mathbf{R}}{ds})$ and the curvature $\kappa(s)$ of the curve at the point s is then given by:

$$\kappa(s) := \left| \frac{d\mathbf{t}}{ds} \right|.$$

The triad $(\mathbf{t}(s), \mathbf{n}(s), \mathbf{b}(s))$ evolves along s according to the Frenet–Serret equations:

$$\frac{d\mathbf{t}}{ds} = \kappa\mathbf{n}(s) \quad \frac{d\mathbf{n}}{ds} = -\kappa\mathbf{t}(s) + \tau\mathbf{b}(s) \quad \frac{d\mathbf{b}}{ds} = -\tau\mathbf{n}(s), \quad (3)$$

where τ is the torsion of the curve $\mathbf{R}(s)$. If the curvature κ and the torsion τ are known for all s then the Frenet–Serret triad can be obtained as unique solution of (3). Next the space curve $\mathbf{R}(s)$ can be reconstructed by integrating the tangent vector $\mathbf{t}(s)$.

A thin rod can be modelled by a space curve $\mathbf{R}(s)$ joining the loci of the centroids of the cross sections together with the local basis $(\mathbf{d}_1(s), \mathbf{d}_2(s), \mathbf{d}_3(s))$ attached to the rod material. This local basis can be expressed through the Frenet–Serret triad as follows:

$$(\mathbf{d}_3(s), \mathbf{d}_2(s), \mathbf{d}_1(s)) = (\mathbf{t}(s), \mathbf{n}(s), \mathbf{b}(s)) \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \phi & -\sin \phi \\ 0 & \sin \phi & \cos \phi \end{pmatrix},$$

where ϕ is the twist angle of the rod. The components of the derivatives of the local basis $(\mathbf{d}_3(s), \mathbf{d}_2(s), \mathbf{d}_1(s))$ with respect to s can be expressed by using the twist vector $\mathbf{k}(s) = \kappa_1\mathbf{d}_1 + \kappa_2\mathbf{d}_2 + \kappa_3\mathbf{d}_3$ as follows:

$$\frac{d\mathbf{d}_i}{ds} = \mathbf{k}(s) \times \mathbf{d}_i(s), \quad i = 1, 2, 3.$$

The static Kirchhoff equations describe the shape of the rod under the effects of internal elastic stresses and boundary constraints, in the absence of external force fields. Let $\mathbf{F}(s)$ is the tension and $\mathbf{M}(s)$ is the torque of the rod. In the approximation of a linear theory (the Hook's law applies) the torque \mathbf{M} is related to the twist vector \mathbf{k} by $\mathbf{M}(s) = \mathcal{S} \cdot \mathbf{k}(s)$, where $\mathcal{S} = \text{diag}(1, a, b)$. The constant a measures the asymmetry of the cross section and b is the scaled torsional stiffness. In particular for symmetric

($a = 1$) hyperelastic ($b = 1$) rods we have $\mathbf{M}(s) = \mathbf{k}(s)$. In the generic case the torque is

$$\mathbf{M}(s) = \kappa_1(s)\mathbf{d}_1(s) + a\kappa_2(s)\mathbf{d}_2(s) + b\kappa_3(s)\mathbf{d}_3(s) \quad (4)$$

and the elastic energy of the Kirchhoff rod is given by:

$$H = \frac{1}{2} \int_{s_1}^{s_2} \mathbf{M}(s) \cdot \mathbf{k}(s) ds = \frac{1}{2} \int_{s_1}^{s_2} (\kappa_1^2(s) + a\kappa_2^2(s) + b\kappa_3^2(s)) ds \quad (5)$$

The conservation of the linear and angular momenta is provided by the static Kirchhoff equations:

$$\frac{d\mathbf{F}}{ds} = 0, \quad (6)$$

$$\frac{d\mathbf{M}}{ds} + \mathbf{d}_3(s) \times \mathbf{F}(s) = 0. \quad (7)$$

Here $\mathbf{F}(s)$ is the tension of the rod and the torque $\mathbf{M}(s)$ is given by (4) and the twist vector reads

$$\mathbf{k}(s) = (\kappa(s) \sin \phi, \kappa(s) \cos \phi, \tau + \phi_s), \quad (8)$$

where the twist angle ϕ is a function of the arc length parameter s : $\phi = \phi(s)$. The expression for the tension $\mathbf{F}(s)$ in the local basis $\mathbf{d}_1, \mathbf{d}_2, \mathbf{d}_3$:

$$\mathbf{F}(s) = F_1(s)\mathbf{d}_1(s) + F_2(s)\mathbf{d}_2(s) + F_3(s)\mathbf{d}_3(s)$$

reduces the Kirchhoff equations (6) and (7) to the following system of ODE's:

$$F_{1,s} + \kappa_2 F_3 - \kappa_3 F_2 = 0 \quad (9)$$

$$F_{2,s} + \kappa_3 F_1 - \kappa_1 F_3 = 0 \quad (10)$$

$$F_{3,s} + \kappa_1 F_2 - \kappa_2 F_1 = 0 \quad (11)$$

$$F_1 = -a\kappa_{2,s} + (b-1)\kappa_1\kappa_3 \quad (12)$$

$$F_2 = \kappa_{1,s} + (b-a)\kappa_2\kappa_3 \quad (13)$$

$$b\kappa_{3,s} + (a-1)\kappa_1\kappa_2 = 0. \quad (14)$$

Using the parameterization of the twist vector (8) from (14) for the case of constant curvature $\kappa(s) = \kappa_0$ we get the famous static (scalar) sine-Gordon equation:

$$\frac{d^2 u}{ds^2} + \frac{(a-1)}{b} \kappa_0^2 \sin u(s) = 0, \quad u(s) = 2\phi(s). \quad (15)$$

This second order differential equation is a completely integrable Hamiltonian system and allows so-called “soliton”-like solutions. It appears in a wide variety of physical problems for e.g. charge-density-wave materials, splay waves in membranes, magnetic flux in Josephson lines, torsion coupled pendula, propagation of crystal dislocations, Bloch wall motion in magnetic crystals, two-dimensional elementary particle models in the quantum field theory, etc.

For a symmetric rod, i.e. $a = 1$ the equation (15) simplifies to $\frac{d^2 u}{ds^2} = 0$, i.e. $\phi_s = \text{const}$. This is the usual case widely discussed in the literature [12]. The cross-section of the symmetric rod ($a = 1$) has a continuous rotational symmetry around the central axis. Therefore the elastic energy density h does not depend on ϕ and from the variational principle it follows that h could be only a function of the derivatives ϕ_s . Therefore the only solution for a constant twist is $\phi_s = \text{const}$.

There have been even attempts to generalize this result to the asymmetric case ($a \neq 1$) [4], i.e. to show that $\phi_s = \text{const}$ holds true for any Kirchhoff rod.

The asymmetric case has been overlooked for a long time. For a constant curvature and torsion along the centre-line it represents another integrable case of the Kirchhoff equations for a thin elastic rod. This opens new possibilities for a more adequate modelling of bio-polymers and gives the phenomenological bases for the widely used DNA models. Here there is no more continuous rotational symmetry of the cross-section around the centre axis and obviously h depends on ϕ as well. So the constant twist is no more a solution.

The solution of (15) is compatible with the full system of Kirchhoff equations (9)–(14) for constant curvature and torsion.

3. The Spin Chain Model

Let us consider the following spin chain model with two perpendicular spins per site: the spin vectors \mathbf{S}_1 and \mathbf{S}_2 have different lengths and are given by

$$\begin{aligned} \mathbf{S}_1(s) &= \mathbf{n}(s) \cos \phi + \mathbf{b}(s) \sin \phi, & \mathbf{S}_1^2 &= 1, & \phi &= \phi(s); \\ \mathbf{S}_2(s) &= -\sqrt{\frac{b-a+1}{a+b-1}} \mathbf{n}(s) \sin \phi + \sqrt{\frac{b-a+1}{a+b-1}} \mathbf{b}(s) \cos \phi, & \mathbf{S}_2^2 &= \frac{b-a+1}{a+b-1}. \end{aligned} \quad (16)$$

Here also both spin vectors are orthogonal: $\mathbf{S}_1(s) \cdot \mathbf{S}_2(s) = 0$ for every s . This is an integrable system with Hamiltonian given by

$$H = J_0 \sum_i (\mathbf{S}_{1,i}(s) \cdot \mathbf{S}_{1,i+1}(s) + \mathbf{S}_{2,i}(s) \cdot \mathbf{S}_{2,i+1}(s)),$$

which in the continuum limit leads to:

$$H = J_0 \int_{s_1}^{s_2} \left[\left(\frac{\partial \mathbf{S}_1}{\partial s} \right)^2 + \left(\frac{\partial \mathbf{S}_2}{\partial s} \right)^2 \right] ds = J_1 \int_{s_1}^{s_2} (b(\tau + \phi_s)^2 + \kappa^2(a-1) \sin^2 \phi) ds,$$

where J_1 is the renormalized coupling constant, $s \in [s_1, s_2]$ and the subscript s means a derivative with respect to s . This Hamiltonian coincides with that one in (5) where $\mathbf{k}(s)$ has been replaced from (8). Thus the asymmetric Kirchhoff rod is mapped onto a two-spin chain. If the curvature is constant $\kappa(s) = \kappa_0$, then the Euler–Lagrange equation gives the (scalar) static sine–Gordon equation:

$$\frac{d^2 \phi}{ds^2} + \kappa_0^2 \frac{1-a}{b} \sin \phi \cos \phi = 0. \quad (17)$$

When $a \rightarrow 1$ the Hamiltonian (17) simplifies to $\int_{s_1}^{s_2} (\tau + \phi_s)^2 ds$, so the Euler–Lagrange

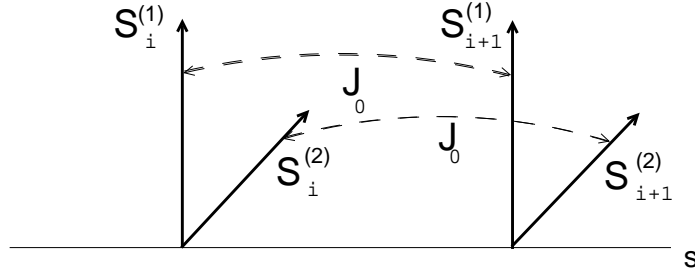


Figure 1. A two-spin XY chain system with a coupling constant J_0 that corresponds to the Kirchhoff rod model.

equation leads to $\phi_{ss} = 0$, or $\phi_s = \text{const.}$ Note that the case $a = 1$ corresponds to a symmetrical Kirchhoff rod. Such a rod-model is mapped onto a symmetrical spin chain system $(\mathbf{S}_1, \mathbf{S}_2)$ with $\mathbf{S}_1^2 = \mathbf{S}_2^2 = 1$. Note that the mapping of the Kirchhoff symmetric rod needs a two-spin XY chain rather than a simple one-spin XY chain. From (17) one can easily get that

$$\left(\frac{d\phi}{ds}\right)^2 + \kappa_0^2 \frac{1-a}{b} \sin^2 \phi(s) = 0,$$

which may be used for the calculation of the corresponding static energy. For the asymmetric thin elastic rod the model Hamiltonian takes the form:

$$H = \int_{s_1}^{s_2} \left((\tau + \phi_s)^2 + \kappa_0^2 \frac{a-1}{b} \sin^2 \phi \right) ds \quad (18)$$

Here we shall discuss in brief the static soliton solutions of the model (18): The kink type solution of the static sine-Gordon equation (15), (17) is given by

$$\phi(s) = 2 \arctan \left[\exp \left(\frac{1}{\kappa_0} \sqrt{\frac{b}{1-a}} s \right) \right], \quad (19)$$

and the corresponding static energy is

$$E_{\text{kink}} = 4\kappa_0 \sqrt{\frac{1-a}{b}} \tanh \left(\kappa_0 \sqrt{\frac{1-a}{b}} l \right) \quad (20)$$

The periodic (soliton lattice) solution of (15), (17) is

$$\phi(s) = 2 \arccos \left[\text{sn} \left(\frac{\kappa_0}{k} \sqrt{\frac{1-a}{b}} s, k \right) \right] \quad (21)$$

with the periodicity $4 \frac{\kappa_0}{k} \sqrt{\frac{1-a}{b}} K(k)$, where k is the modulus of the Jacobian elliptic function sn (sine amplitude), and $K(k)$ is the complete elliptic integral of the first kind. In the limit $k \rightarrow 1$ we have $K(k) \rightarrow \infty$ and the half-period tends to infinity as well, so we recover the single kink soliton solution (19).

The corresponding static energy per soliton of the soliton lattice is given by:

$$E_{\text{soliton}} = \frac{\kappa_0}{k} \sqrt{\frac{1-a}{b}} \left(E(k) - \frac{1}{3} (k')^2 K(k) \right), \quad (22)$$

where $E(k)$ is the complete elliptic integral of second kind. In the single soliton limit ($k \rightarrow 1$) the lattice energy per soliton (22) reduces to eqn. (20).

4. Conclusions

We have shown that the single asymmetric elastic Kirchhoff rod model can be mapped onto a 2-spin XY Heisenberg chain and the spin vectors must have different lengths. In this case the Euler-Lagrange equation for the spin chain Hamiltonian gives the static sine-Gordon equation. For the case of symmetric rods ($a = 1$) both spins have the same length. The symmetric ($a = 1$) and the asymmetric ($a \neq 1$) Kirchhoff rods have very different static properties. In general the family of thin elastic Kirchhoff rods falls into two groups: i) the group of symmetric rods ($a = 1$). Here the twist is constant along the rod and if the torsion is constant as well, the Kirchhoff equations are integrable and the curvature satisfies the non-linear Schrödinger equation; ii) the

group of asymmetric rods ($a \neq 1$). Here in general the twist and the curvature satisfy a coupled differential equations (for a constant torsion). In the special case where the curvature is constant the system of Kirchhoff equations is integrable again and the twist satisfies the sine-Gordon equation.

The dynamics of such models, which is of interest for realistic biopolymers, should be investigated. Due to the Galilean invariance of the sine-Gordon equation (15) a special class of dynamical travelling wave type solutions can be obtained from the static ones by Galilean boost.

The general assumption that all thin rods exhibit constant twist should now be restricted to the class of symmetric thin rods only and to all straight rods as well. The class of asymmetric thin rods does not belong to this category. Here the twist is not constant and “interacts” with the curvature. In the case of constant curvature, the problem has exact solution. For non-constant curvature the case is more complex and should be of considerable interest e.g. for the problem of DNA supercoiling [13, 14, 15, 16, 17, 18].

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